Populations

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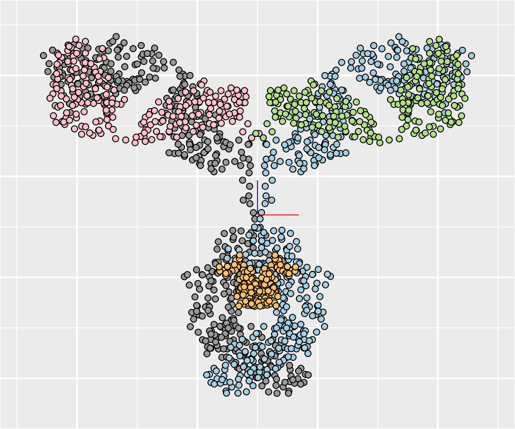
Problem: Structure of human immunoglobulin G1 (IgG1)

Recall exploring how the geometry of the human immunoglobulin G1 molecule related to different variables associated with each “alpha” carbon.



E.g. here, colours are assigned to each carbon atom according to the value of its `chainID` variable.

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The data frame `igg1` (from the package loon.data) has 1556 rows, one for each alpha carbon. In the above notation, we can take

- row i to be the ith unit in $\mathcal{P}$, and
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- they can also be thought of as possible **keys** to identify identical units (e.g. as `linkingKeys` in `loon` plots).

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Notation: Populations will be distinguished from one another by using subscripts as in $\mathcal{P}_{IgG1}$.

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The data frame `igg1` also has 10 columns, each being a variable recording its value for every individual alpha carbon (unit) in the data frame.

For example, the three dimensional geometric location of the ith alpha carbon is recorded as the ith value of the variables `x`, `y`, and `z`.

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- similarly, the other two coordinates of the 3D locations $y(u)$ and $z(u)$ (or simply y_u and z_u) are also *continuous* and *ratio scale* variates.

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- e.g. a variate such as $preference(u) \in \{"hate", "dislike", "neutral", "like", "love"\}$
- there are no strictly ordinal variates in the `igg1` data (though several, *residueSequenceNum*, x, y, and z can each be ordered)

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Data: Realizations, observations, and variates

The first three rows of `igg1` are

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head(igg1, n=3)
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##   recordType name residue chainID residueSequenceNum       x      y       z
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## 2       ATOM   CA     VAL       H                  2 -60.766 48.666 -15.351
## 3       ATOM   CA     GLN       H                  3 -57.145 48.577 -16.631
##     residueName                    group
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## 2        Valine Non-polar (hydrophobic)
## 3     Glutamine       Polar (uncharged)
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Data: Realizations, observations, and variates

The first three rows of igg1 are

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```

```
##   recordType name residue chainID residueSequenceNum       x      y       z
## 1       ATOM   CA     GLU       H                  1 -62.259 45.262 -16.149
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N.B. Some people refer to this standard arrangement and interpretation as a **tidy data** representation.

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prop <- with(igg1, sum(recordType == "HETATM") / length(recordType))
paste0(round(100 * prop), "%") # as a character string for printing
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## [1] "14%"
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## [1] "14%"
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Or, maybe, a two way table of counts for combinations of `chainID` and `group`

```
knitr::kable(with(igg1, table(chainID, group)))
```

	Acidic	Basic	Non-polar (hydrophobic)	Polar (uncharged)	Sugar
C	0	0	0	0	220
H	38	54	171	189	0
I	38	54	171	189	0
L	17	19	78	102	0
M	17	19	78	102	0

where some similarities and differences between chains are immediately apparent.

Chains `H` and `I` are "heavy", `L` and `M` "light", and `C` is a carbohydrate chain.

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Alternatively, **graphical attributes** can sometimes provide complex summary information in a meaningful and comprehensible way.

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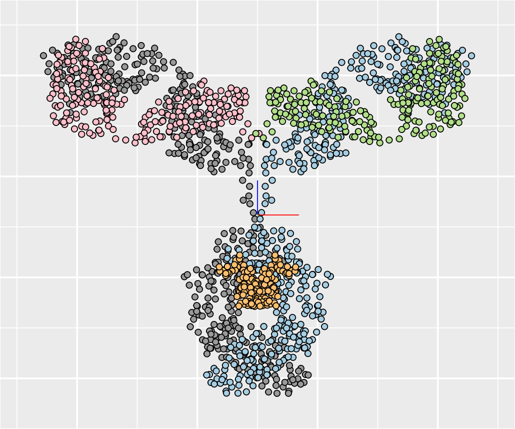
For example, as already seen, the geometric locations shown in an interactive 3D scatterplot can be very informative (here coloured by chain ID):



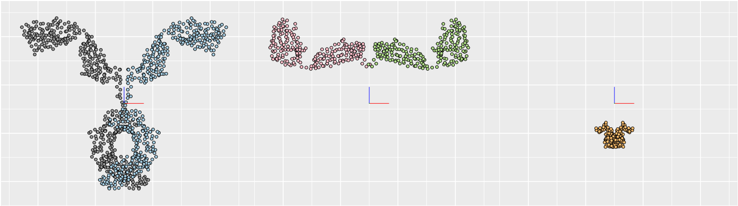
Population attributes – graphical

Interactive graphics, as in loon , make it very easy to construct informative graphical attributes by direct manipulation, as well as to save them for traditional publication:

```
heavyChain <- (igg1$chainID == "H") | (igg1$chainID == "I")
lightChain <- (igg1$chainID == "L") | (igg1$chainID == "M")
carbs <- (igg1$chainID == "C")
p3d["active"] <- heavyChain
p3d_heavy <- plot(p3d, draw = FALSE)
p3d["active"] <- lightChain
p3d_light <- plot(p3d, draw = FALSE)
p3d["active"] <- carbs
p3d_carbs <- plot(p3d, draw = FALSE)
# And plot these using grid graphics extra functionality
library(gridExtra)
# to arrange them in sequence
grid.arrange(p3d_heavy, p3d_light, p3d_carbs, nrow = 1)
```

Population attributes – graphical

The three groups of chains, heavy, light, and carbohydrate:



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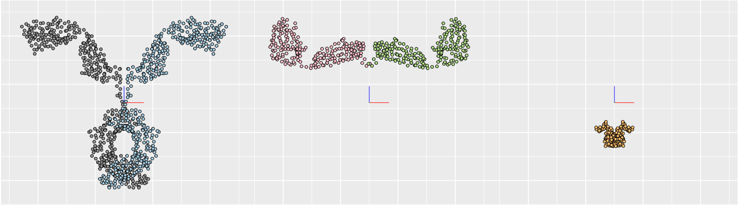

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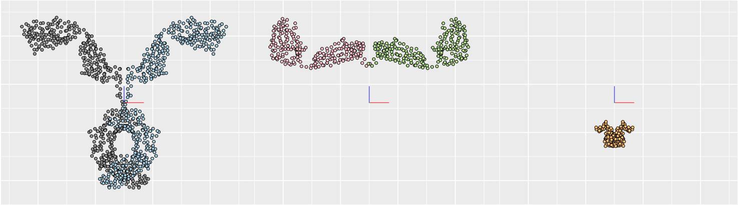

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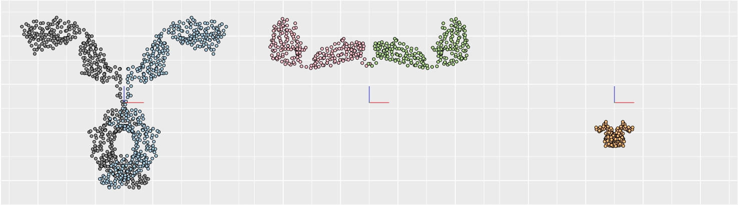

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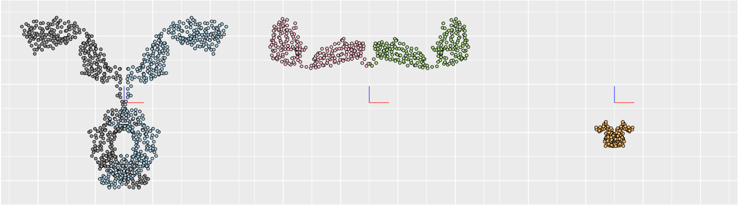

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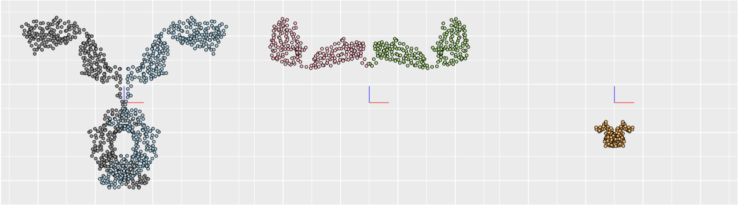

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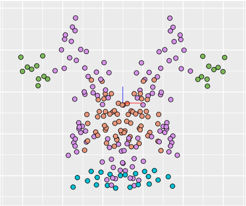
3. $u \in \{u \;:\; u \in \mathcal{P}$ and $chainID(u) = "C"\}$.

Where $chainID(u)$ values are encoded by colour.

Population attributes – graphical

Or possibly zoom in on the carbohydrate chain coloured by `residue`:

```
p3d["active"] <- carbs
l_scaleto_active(p3d)
p3d["color"] <- igg1$residue
p3d["size"] <- 10
plot(p3d)
```



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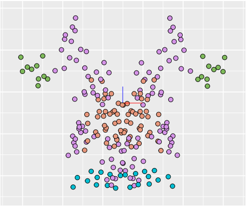

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In either case, an attribute is a summary of $\mathcal{P}$ and as such it will always be of interest to examine how the well it does and does not describe all of the units it targets in its summary.

Quick numerical attributes

Some simple attributes are easily had (and are worth checking as a habit):

```r
summary(igg1)
```

```
##   recordType        name         residue     chainID residueSequenceNum
##  ATOM   :1336   CA      :1336   SER    :178   C:220   Min.   :  1.0
##  HETATM: 220    C1      :  18   VAL    :122   H:452   1st Qu.: 85.0
##                 C2      :  18   NAG    :112   I:452   Median :279.5
##                 C3      :  18   THR    :106   L:216   Mean   :301.2
##                 C4      :  18   PRO    :102   M:216   3rd Qu.:522.0
##                 C5      :  18   GLY    : 98           Max.   :716.0
##                 (Other): 130   (Other):838
##        x                   y                 z
##  Min.   :-71.18000   Min.   :-65.93   Min.   :-27.45500
##  1st Qu.:-17.32575   1st Qu.:-23.17   1st Qu.: -9.69500
##  Median : -0.01650   Median : 35.71   Median :  0.01050
##  Mean   : -0.00268   Mean   : 16.56   Mean   :  0.00856
##  3rd Qu.: 17.30550   3rd Qu.: 52.65   3rd Qu.:  9.68825
##  Max.   : 71.20500   Max.   : 75.38   Max.   : 27.52100
##
##             residueName                         group
##  Serine             :178   Acidic                  :110
##  Valine             :122   Basic                   :146
##  N-acetylglucosamine:112   Non-polar (hydrophobic):498
##  Threonine          :106   Polar (uncharged)       :582
##  Proline            :102   Sugar                   :220
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```

Each variate is given its own two columns of `name : value` pairs.

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##  Threonine          :106   Polar (uncharged)       :582  
##  Proline            :102   Sugar                   :220  
##  Glycine            : 98                                 
##  (Other)            :838                                 
```

Each variate is given its own two columns of `name : value` pairs.

- Categorical variates show counts of values.

Quick numerical attributes

Some simple attributes are easily had (and are worth checking as a habit):

```r
summary(igg1)
```

```
##   recordType        name         residue     chainID residueSequenceNum
##  ATOM  :1336   CA      :1336   SER    :178   C:220   Min.   :  1.0     
##  HETATM: 220   C1      :  18   VAL    :122   H:452   1st Qu.: 85.0     
##                C2      :  18   NAG    :112   I:452   Median :279.5     
##                C3      :  18   THR    :106   L:216   Mean   :301.2     
##                C4      :  18   PRO    :102   M:216   3rd Qu.:522.0     
##                C5      :  18   GLY    : 98           Max.   :716.0     
##                (Other): 130   (Other):838                             
##        x                   y                 z            
##  Min.   :-71.18000   Min.   :-65.93   Min.   :-27.45500  
##  1st Qu.:-17.32575   1st Qu.:-23.17   1st Qu.: -9.69500  
##  Median : -0.01650   Median : 35.71   Median :  0.01050  
##  Mean   : -0.00268   Mean   : 16.56   Mean   :  0.00856  
##  3rd Qu.: 17.30550   3rd Qu.: 52.65   3rd Qu.:  9.68825  
##  Max.   : 71.20500   Max.   : 75.38   Max.   : 27.52100  
##                                                          
##               residueName                      group    
##  Serine             :178   Acidic                 :110  
##  Valine             :122   Basic                  :146  
##  N-acetylglucosamine:112   Non-polar (hydrophobic):498  
##  Threonine          :106   Polar (uncharged)      :582  
##  Proline            :102   Sugar                  :220  
##  Glycine            : 98                                
##  (Other)            :838                                
```

Each variate is given its own two columns of `name : value` pairs.

- Categorical variates show counts of values.
- Numeric variates show traditional summary statistics of that variate's values.

Where's Waldo? Numerical attributes

What can we learn about the distribution of the values of these variates from these numbers?

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Exercise: consider what happens to each of these measures when any variate y is transformed to $z = ay + b$ for two non-zero constants a and b.

Quick graphical attributes

Similarly, in R , simple graphical attributes are also easily had (and worth checking as a habit).

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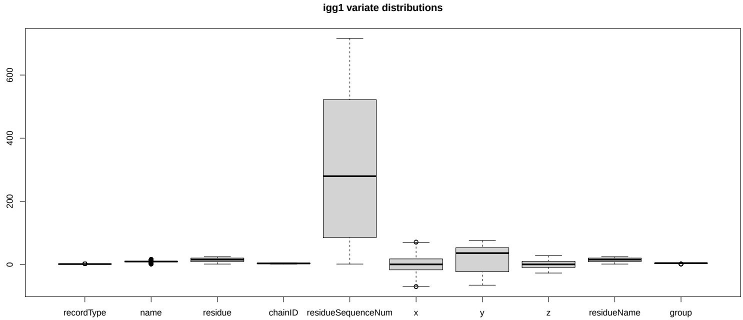
```
boxplot(igg1, main = "igg1 variate distributions", col = "lightgrey")
```



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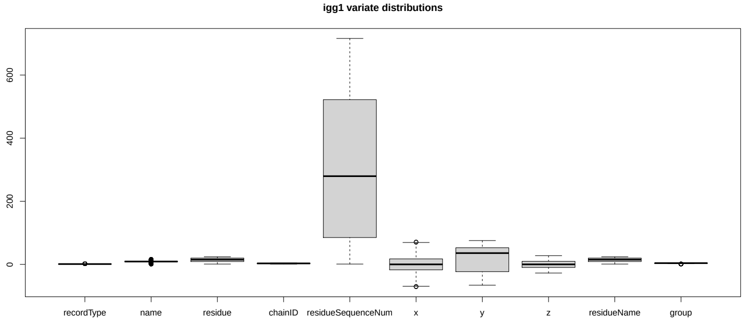

Which is not that informative for most of the variates since they are categorical and boxplots are designed for continuous variates. Nevertheless, like summary() it gives a quick sense of the variates and the extent of their values.

There are other displays better suited to categorical variates.

Graphical attributes for categorical variates

Similarly, we might look at graphical attributes to summarize the distribution of values for each categorical variate.

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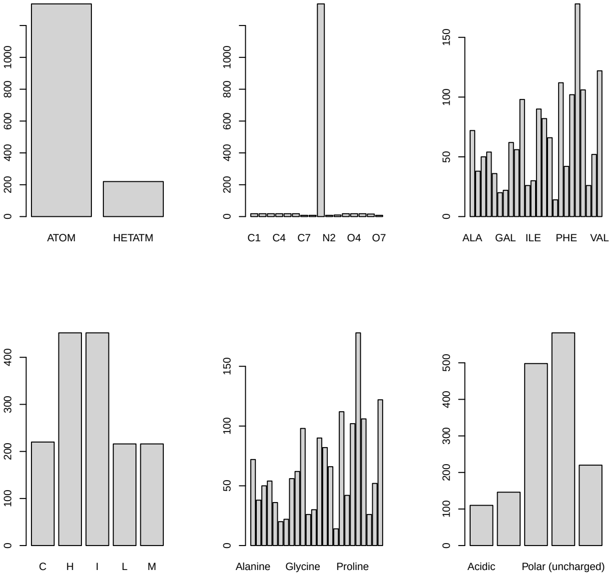
A bar plot for each:

```
isCatVar <- sapply(names(igg1), FUN  = function(name) is.factor(igg1[,name]))
catVars <- names(igg1)[isCatVar]
nrows <- floor(sqrt(length(catVars)))
ncols <- ceiling(sqrt(length(catVars)))
savePar <- par(mfrow = c(nrows, ncols))
for (var in catVars) {
    counts <- summary(igg1[,var])
    vals <- levels(igg1[,var])
    barplot(counts, names.arg = vals, col="lightgrey")
}
par(savePar)
```

Graphical attributes for categorical variates

A bar plot for each:



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Interactive graphical attributes for categorical variates

For exploratory work, it would be better if these were interactive.

```
isCatVar <- sapply(names(igg1), FUN  = function(name) is.factor(igg1[,name]))
catVars <- names(igg1)[isCatVar]
# Could simply have each plot in a separate window
# or in a single window as shown here
nrows <- floor(sqrt(length(catVars)))
ncols <- ceiling(sqrt(length(catVars)))

barplotWindow <- tktoplevel()   # THE WINDOW
row <- 0
col <- 0
for (var in catVars) {
    barplot <- l_hist(igg1[,var],
                      linkingGroup = "igg1",
                      title = var,
                      parent = barplotWindow)
    if (col >= ncols){
        row <- row + 1
        col <- 0}
    tkgrid(barplot, row = row, column = col, sticky = "nesw")
    col <- col + 1}
# Configure columns to resize with window
for (col in 0:(ncols-1)){tkgrid.columnconfigure(barplotWindow, col, weight = 1)}
# Configure rows to resize with window
for (row in 0:(nrows-1)){tkgrid.rowconfigure(barplotWindow, row, weight = 1)}
# Add a title
tktitle(barplotWindow) <- "Counts for factors"
```

Quick graphical attributes - two dimensional

In R , there are also simple graphical attributes easily had for pairs of variates (and worth checking as a habit, provided there aren't too many).

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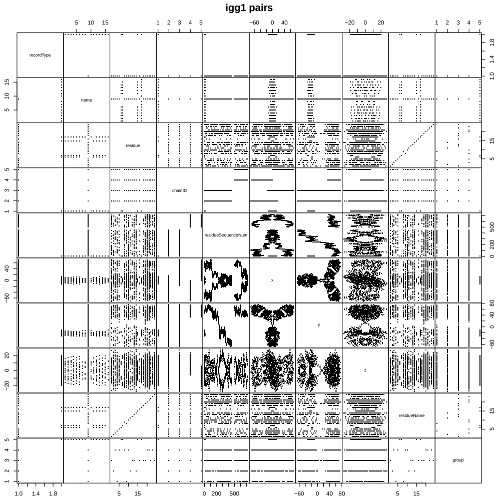
```
plot(igg1, gap = 0, pch = ".", col = "black", main = "igg1 pairs")
```



Might be better to restrict consideration just to those that variates that are not factors.

Quick graphical attributes - two dimensional interactive

An interactive version is available in loon via `l_pairs()`

Quick graphical attributes - two dimensional interactive

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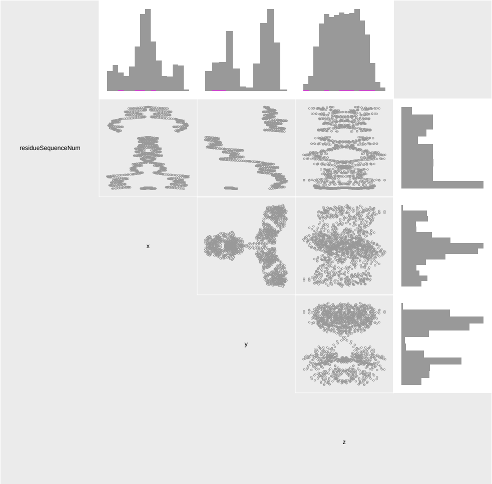
```
isCtsVar <- sapply(names(igg1), FUN  = function(name) !is.factor(igg1[,name]))
ctsVars <- names(igg1)[isCtsVar]
pp <- l_pairs(igg1[,ctsVars], glyph = "ocircle", size = 1,
              showHistograms = TRUE,
              linkingGroup = "igg1",  title = "Continuous pairs")
plot(pp)
```



Problem - Visible minorities in Canada 2006

Recall the `minority` data from loon.data.

Questions:

- What are the units u?

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